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Method of Fractional Derivatives in Time-Dependent Diffusion

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1. Introduction

Many theoretical problems of diffusion lead to the solution of the initial boundary-value problem

$$\partial_t u - \alpha_2(x,t)\partial_x^2 u - \alpha_1(x,t)\partial_x u + \alpha_0(x,t)u = 0 \quad \text{in} \quad \Omega \tag{1}$$

$$u\big|_{t=0} = 0\,,\; u\big|_{x=0} = \varphi(t),\; u\big|_{x\to\infty} \to 0\,, \tag{2}$$

where $\Omega = (0,\infty)\times(0,\infty)$ and for the sake of simplicity we assume that $\varphi(t)$ is a continuous function and $\alpha_k(x,t) \in C^\infty(\Omega)$ ($k = 0,1,2$) with $\alpha_2(0,t) \neq 0$.

It is well known that the exact analytical solution to the problem (1), (2) is often difficult if not impossible to obtain. However, particularly for diffusion-limited reactions, the value of the local flux on the boundary proportional to the function $j_\infty(t) = -\partial_x u\big|_{x=0}$ is of main interest. It turned out that one can find the function of interest $j_\infty(t)$ without knowing the solution of the posed problem using the method of fractional derivatives (MFD) suggested by Babenko

$$j_\infty(t) = \sum_{n=0}^{\infty} f_n(t)\,\partial_t^{\frac{1-n}{2}} \circ \varphi(t)\,. \tag{3}$$

Here $f_n(t) = a_n(0,t)\big/\sqrt{\alpha_2(0,t)}$, where $a_n(x,t)$ are functions to be determined from the recurrent relations obtained with the help of the corresponding operator equation; $\partial_t^{\frac{1-n}{2}}$ are operators of fractional differentiation with respect to time and defined by the following formula

$$\partial_t^\mu \circ g(t) = \frac{1}{\Gamma(1-\mu)}\frac{d}{dt}\int_0^t (t-\tau)^{-\mu} g(\tau)\,d\tau\,,\; \mu \in (-\infty,1)\,,$$

where $\Gamma(z)$ is the gamma function.

2. Method validation and some applications

However, so far the range of validity of expansion (3) was unknown. We established the convergence radius of the functional series (3):

$$R = q^{-2}\text{, where } q = \overline{\lim_{k\to\infty}} \sqrt[k]{\left\| a_k\left(x,t\right)\right\|_\infty \left\|\varphi\left(t\right)\right\|_\infty}\ .$$

Moreover, a useful uniform upper bound for the solution $u\left(x,t\right)$ in an important particular case when $\alpha_2\left(x,t\right)\equiv 1$, $\alpha_1\left(x,t\right)\equiv 0$ was proved. Using the MFD we also found the exact connection between the function $j_\infty\left(t\right)$ and the function $j_h\left(t\right) = -\partial_x u_h\big|_{x=0}$ corresponding to the initial boundary-value problem (1), (2) with $u \to u_h$ and more general Robin's boundary condition at $x = 0$, i. e.

$$-\partial_x u_h\big|_{x=0} = h\left[\varphi\left(t\right) - u_h\left(0,t\right)\right]\text{, where } h \text{ is a positive constant:}$$

$$j_h\left(t\right) = j_\infty\left(t\right) - \frac{1}{h}\frac{d}{dt}\int_0^t j_\infty\left(t-\tau\right) j_h\left(\tau\right) d\tau\ . \tag{4}$$

We also applied the MFD to the very important particular case of diffusion-controlled reactions between ions. In this case $\alpha_0\left(x,t\right)\equiv 0$, $\alpha_1\left(x,t\right)\equiv 1$, $\alpha_2\left(x,t\right)\equiv \frac{2}{x}\left(1-\frac{\beta}{x}\right)$, where $\beta = \mu r_c/2R$, r_c is the Onsager length [1], $\mu < 0\left(>0\right)$ for attraction (repulsion). For the attractive potentials the MFD gives

$$j_\infty\left(t;\beta\right) = \left(1+\frac{1}{\sqrt{\pi t}}\right)\exp\left(-\beta^2 t\right) - \beta\,\mathrm{erfc}\left(\beta\sqrt{t}\right) + O\left(\frac{1}{\beta}\right) \quad \text{as } \left|\beta\right| \to \infty \text{,} \tag{5}$$

where $t = t/t_D$, $t_D = R^2/D$ is the characteristic relaxation time for pure diffusion, R is the reaction radius and D is the sum of the diffusion coefficients for ions. We proved that, contrary to what we have assumed before, the characteristic relaxation time for the attractive Coulomb potential is less than t_D and has the form

$$t_r\left(\beta\right) = \left[\exp\left(2\beta\right)-1\right]^2 t_D \big/ 4\beta^2\ . \tag{6}$$

Finally, with the aid of the MFD, we calculated the correction for the effect of the hydrodynamic interaction on the diffusion-controlled rate coefficient.

3. Conclusion

The rigorous proof for validity of the method of fractional derivatives is presented. Using this method we found the relationship between the diffusion flux in the case of the Dirichlet and Robin boundary conditions. Application of the method of fractional derivatives to diffusion-controlled reactions between ions allows us to derive an analytical formula for the total diffusive flux, the corresponding realaxation time and the correction for the effect of the hydrodynamic interaction.

References

[1] S.A. Rice, Diffusion-limited Reactions, Elsevier, Amsterdam, 1985.